Vortex structures in few-electron quantum dots with spin degree of freedom

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The vortex structures and formations of the few-electron states in quantum dots without the Zeeman splitting are investigated. With spin degree of freedom, it is noticed that both the choices of probe electron and the ways to fix the other electrons in conditional single-particle wave functions affect the display of the vortex structures and behaviors. Then the vortex transitions in magnetic fields for the lowest states with different spins are studied. When the field is not very strong, with the increase of the field, the vortex number is monotone non-decreasing, and there are absent states although their angular momenta are in accordance with transition rules given by the theory of electron molecules. Different behaviors of the vortices with the change of interaction range reveal the respective analogies to the vortices of electrons and quasi-particles in fractional quantum Hall system. The separated vortices keep apart from the electrons even when the interaction is screened and such behavior can give an understanding of the absences of the angular momenta in the transition sequences.

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I. INTRODUCTION

The formation and distribution of vortices¹ are important aspects in the studies of many-body systems, such as superconductors and Bose-Einstein condensates. The vortices can give the information of the many-body wave functions and the correlations between particles. The famous Laughlin wave function² whose vortices are concentrated on the electron is the basis to understand the fractional quantum Hall effect (FQHE) of two-dimensional electron gas (2DEGs) in strong magnetic fields. The concentrated vortices keep the electrons far apart and reduce the short-range interaction most effectively. When an electron moves around a vortex, the phase of the manybody wave function will be changed by $2n\pi$, where n is the order of the zero. In composite fermion theory³ where the FQHE can be understood in terms of its integer counterpart, the electron feels the effective magnetic field because the phase change caused by the vortices partly cancels the Aharonov-Bohm phase caused by the field.

The quantum dots (QDs) with a few electrons have attracted a lot of interests in recent years. In magnetic fields, the quantum dots can be viewed as the precursor of quantum Hall system. So called maximum density droplet (MDD) which corresponds to the filling factor $\nu = 1$ has been demonstrated by both the experiments and theoretical studies. Besides these, the electron transport experiments in magnetic fields have shown various transitions of the charge distributions.⁴ This leads to the increasing interests in investigations of the electronic states and vortices.^{5,6} The long-range part of the interaction is more important in quantum dots. When $\nu < 1$, it has been found that the vortices are no longer concentrated on but bounded around the electrons.^{5,7} The interaction also makes the liquid-crystal transition^{8,9,10} in quantum dots much easier than that in 2DEGs. With

the localization of the electrons, the distributions of vortices become more dispersed to form the vortex clusters.

Due to the Zeeman splitting, the electrons are taken as full polarized in most theoretical discussions on ground states of QDs in strong fields. Then the spin degree of freedom can be ignored and is irrelevant to the studies of vortices. With the improvements of nanotechnology, it is recently achieved to fabricate the QDs with negligible Zeeman splitting. 11,12 Then even in the strong magnetic fields, the spin degree of freedom should be taken into account when the properties of the ground and low lying states are concerned. The angular momentum transitions of the ground states and the lowest states with different spins for a few electrons in quantum dot have been explored by both the theory of electron molecules 13,14 and the exact diagonalization. 15,16 The formation and redistribution of the vortices with spin degree of freedom are important aspects of understanding the characters of the electronic states and the transport measurements in the system without the Zeeman splitting. In this paper, we study the vortices in few-electron quantum dots with spin degree of freedom to explore the transitions of the electronic states in magnetic fields.

II. CONDITIONAL WAVE FUNCTION WITH SPIN

The model Hamiltonian of a few-electron quantum dot in the magnetic field with parabolic confinement and without the Zeeman splitting is

$$H = \sum_{i=1}^{N} \left[\frac{1}{2m} \left(\hat{P}_i + e\vec{A} \right)^2 + V(r_i) \right] + \sum_{i < j} \frac{e^2}{4\pi\varepsilon |\vec{r}_i - \vec{r}_j|}.$$
 (1)

where N is the particle number, \vec{A} is the vector potential of the field, $V(r_i)$ is the confinement of the dot with

the strength equals to 2meV in the following discussions, and the last term is the Coulomb interaction between particles. The effective mass m of the electron and the static dielectric constant ε are respectively $0.067m_e$ and 12.4 for GaAs. The eigenstates Ψ of the Eq.(1) are obtained by the exact diagonalization. Without the spinorbit coupling, such states are the common eigenstates of the total angular momentum L, the total spin S and its z-component S_z , so in the following discussions we use the abbreviation (L, S, S_z) to represent them.

It has been demonstrated that the vortex structures depend on the range of the interaction between electrons. 17 So we also use the Yukawa screened Coulomb interaction 17,18

$$I(r) = \frac{e^2}{4\pi\varepsilon} \frac{\exp(-r/\alpha)}{r} \tag{2}$$

instead of the Coulomb interaction to understand the vortex behaviors in some of the following discussions.

Having got the many-body eigenstates, we employ the conditional single-particle wave function⁵ with spin degree of freedom to explicitly show the vortices of the wave functions

$$\psi_c(\mathbf{r}) = \frac{\Psi(\mathbf{r}, \sigma^*, \mathbf{r_2}^*, \sigma_2^*, \cdots \mathbf{r}_N^*, \sigma_N^*)}{\Psi(\mathbf{r}^*, \sigma^*, \mathbf{r_2}^*, \sigma_2^*, \cdots \mathbf{r_N}^*, \sigma_N^*)}$$
(3)

where σ_i represent the spins of electrons. In the function, an electron is chosen as the probe electron and other electrons are pinned at fixed positions. In Eq.(3), the variables with asterisk superscript are fixed ones. The phase angle of the conditional wave function reveals the change of the phase of a many-body function when an electron moves around another one. Then the plot of the electron density and the phase of the conditional wave function gives the picture of vortices in the many-body wave function.

We should present some explanations about the choices of the probe and pinned electrons. First, when there are asymmetry between the spin-up and spin-down electrons in some states, the different choices of the probe electron's spin may result in different displays of the vortices. In Fig.1, we present the vortices of the four-electron state (-15.1.1) as an example. We fix the pinned electrons at the most probable radius. The state (-15,1,1) contains three spin-up and only one spin-down electrons. Then there are two choices of the probe electron and they lead to different displays of the vortices. If the probe electron is the spin-up one, it can be seen that there are respectively three and two vortices around each spinup and spin-down fixed electron. If the unique spindown one is chosen to be the probe electron, only two vortices around each spin-up electron can be seen. In the case of the FQHE where the vortices are concentrated on the electrons, Halperin¹⁹ has suggested a set of trial functions including the spin degree of freedom. The polynomial parts of the functions have the form $\prod_{i>j} (z_i - z_j)^{m+1} \prod_{i>j} (\xi_i - \xi_j)^{m-1} \prod_{i,j} (z_i - \xi_j)^n$ where z and ξ are the complex coordinates of the spin-up and

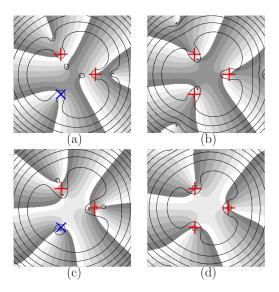


FIG. 1: (Color online) The vortices for the four-electron state (-15,1,1) with a spin-up (left column) and spin-down (right column) probe electron in conditional single-particle wave function. The upper and lower rows correspond to the case where the Coulomb and the screened interactions are adopted, respectively. The density of the probe electron is plotted as contours in logarithmic scale. The phase changes from $-\pi$ to π as the shadowing changes from the darkest gray to white. + and \times indicate the positions of pinned spin-up and -down electrons, respectively.

spin-down electrons. It can be found that the orders of the vortices indeed depend on the spins of the electrons. And from the viewpoint of the electron with a certain species of spin, only parts of the vortices are visible. In the case of the quantum dot, although the vortices are no longer concentrated on the electrons, the number of the visible vortices can still depend on the spins. Nevertheless, with appropriate choice of the spin of the probe electron, we can get useful information about the vortices of a state. In the following discussions about four-electron states, we mainly focus on the ones with $S_z=0$ then there are no such difficulty. For five-electron case with $S_z=0.5$, we chose a spin-up electron as the probe one.

Another feature should be pointed out here is that there are vortices in the system which originate from long-range interactions. And such vortices will move to the infinity if the interactions is totally screened. ¹⁷ In Fig.1b we can see two such vortices. It can be seen in Fig.1d that they will move away when the interaction is screened.

Besides the choice of the probe electron, the manner of the pinned electrons may also affect the vortex displays of some states if there are more than one way to fix the positions of the electrons with spins. For instance, if one spin-up electron is selected as the probe electron for a five-electron state with $S_z=0.5$, and the remainder electrons are fixed at the vertices of a square, there are two inequivalent ways to determine the spin of each pinned

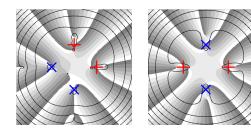


FIG. 2: The vortex displays of the five-electron state (30,0.5,0.5) with the electrons are fixed in the neighbor (a) and alternative (b) modes, respectively. + and \times indicate the positions of pinned spin-up and -down electrons, respectively.

electron, i.e. fix the electrons with same spin at neighbor or alternative positions (we call them neighbor and alternative mode respectively). Then for the states with some angular momenta, the two ways may give different vortex numbers. In Fig.2 there is an example of such situation. With two fixation modes, the displayed vortex numbers of the state (-30,0.5,0.5) are different by one. Such phenomenon will generally occur when we inspect a higher dimensional object from a lower dimensional space, i.e. the visibility of an entity relies on the viewpoint of the projection. It should be pointed out that such differences only exist in the non-full-polarized states. For the fullpolarized states, the spin and spatial parts of the wave functions can be separated and the ways to fix the electrons with different spins do not affect the display of the vortices. For four electron case, there is only one way to fix the electrons if they are fixed at the vertices of an equilateral triangle and of course no such kind of difference exist. Then in the following counts of the vortices of five-electron states with $S_z = 0.5$, we can simply use appropriate fixation mode which give larger vortex number for each state. However, when we discuss the behaviors of the vortices in the subsection III.B, we must inspect the different displays of the vortices more carefully and we will recall this topic there.

III. DISSCUSSION

A. Energy level structures and spin-dependent vortices

Before the detailed study of the vortices, we must discuss the energy level structures of quantum dots briefly. In Fig.3 we show typical energy spectra of four and five electron in magnetic fields obtained from the exact diagonalization. If the Zeeman splitting is concerned, the ground states of the few-electron quantum dot are full-polarized with maximum S_z in strong magnetic fields. With the increase of the field, for the four- and five-electron case there are angular momentum transitions of the ground states whose increment between neighbor

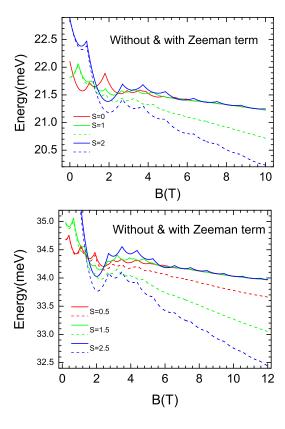


FIG. 3: The energy level of the lowest states with different spins for four-electron (a) and five-electron (b) cases as functions of magnetic fields. The solid and dashed lines correspond to the energies without and with the Zeeman splitting. The N times of the energy of the first landau level have been subtracted from the total energy.

states equals to the particle numbers. The allowable angular momenta are so called "magic number". If the Zeeman splitting can be ignored, the states with same L and S but different S_z are degenerate. The ground states even in strong fields no longer need to be full-polarized and the lowest states with different spins gradually form a narrow band. In the narrow band, the energies of different spin states are nearly degenerate. The ground states in the field corresponding to the fractional filling factor $\nu=1/(2p+1)$ are still full-polarized although they are multiple degenerate due to different S_z . Along with the gradual formation of the narrow band, there are transition from the liquid to crystal states.

With the increase of the field, there are also respective angular momentum transitions for different spin states. The angular momentum rules for the allowable states which can emerge in the transition sequences can be obtained from the electron molecules theory in strong fields^{13,14} or the exact diagonalization. The exact diagonalization also reveals that some states whose angular momenta are in accordance with the rules can be absent from the transition sequence when the electronic states are still liquidlike. With the transition from the liquid to crystal states, the absences gradually disappear. For

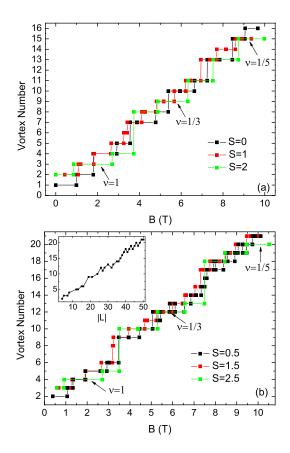


FIG. 4: (Color online) The vortex numbers of the lowest states with different total spins as functions of the magnetic fields. For four-electron case (a), $S_z = 0$ and the black, red and green lines correspond to the states with S = 0,1 and 2, respectively. For five-electron case (b), $S_z = 0.5$ and the black, red and green lines correspond to the states with S = 0.5, 1.5 and 2.5, respectively. The vortex numbers of the states with S = 0.5 as function of the angular momenta are shown in the inset for clarity.

four- and five-electron states, the transition rules and the absent states are listed in Appendix. In the four-electron case, only two states are absent from the transition sequences because the magnetic field can easily make the electrons form rotating Wigner molecules with such a small particle number. However, in the five-electron case, the absences are much more and only disappear in strong fields.

In the transitions, the absolute values of the angular momenta increase. The vortices also gradually increase. We illustrate the vortex numbers of the lowest states with different S and the lowest S_z in Fig.4. The complete data are listed in the Appendix. In the counts, the vortex numbers are those displayed by the conditional wave functions and the vortices which move to the infinity with screened interaction are excluded. The vortex numbers of full-polarized states increase monotonously. And although there are degenerations due to different S_z , the vortices of full-polarized states with different S_z have no

differences. So in the following discussions we will focus on the states with lower S. It can be seen that the vortex numbers in the transition sequences of the nonfull-polarized states are monotone non-decreasing when the magnetic field is not very strong, for five-electron case $\nu \gtrsim 1/3$, i.e. $|L| \lesssim 30$. Such monotonicity is not preserved when the field becomes strong, especially the five-electron case, see also the inset of Fig.4b where the vortex numbers as the function of |L| are shown for clarity. By inspecting the vortices of all the states whose angular momenta are in accordance with the transition rules, it is found that the vortex numbers of five-electron states with L = 6, 11, 14, 20, 23, 31 and S = 0.5 exceed those of the next neighbor ones. And they are absent from the transition sequence to avoid the breakdown of the monotonicity of the vortex number with respect to the field or the angular momentum. There are also other absent states whose total vortex numbers do not break the monotonicity, in the next subsection, we will analyze the vortex distributions and discuss the absences more in-depth.

B. Insight of the vortex formation

In 2DEGs, if the spin degree of freedom is taken into account, when the magnetic field deviates from the values corresponding to the fractional filling factors, the total spin of the ground state is no longer full polarized. Along with the changes of the total spin, there are also quasi-particle (quasi-electron or -hole) excitations, namely the reversed-spin quasi-particle excitations^{20,21} or skyrmions. These excitations will change the manybody wave functions and be reflected in the formations and redistributions of vortices. However, due to the long range Coulomb interaction, the vortices in QDs are dispersed. Especially when the electrons form the RWMs states, the vortices will spread over the whole area. So we employ the Yukawa screened Coulomb interaction¹⁷ to clearly show the origins and behaviors of different vortices in QDs.

In Fig.5 we show the vortex distributions of some states as examples. First kind of states is the ones corresponding to the fractional filling factor 1/(2p+1), like the four-electron state with L=-18 and S=2 whose filling factor is 1/3. Such states with different S_z have same vortex distribution as shown in Fig.5 where the state (-18,2,0) is taken as an example. By the consideration of the screened Coulomb interaction, the dispersive vortices can approach the positions of electrons. This is just the scenario of the Laughlin limit in 2DEGs.

When the field deviates from the value corresponding to the fractional filling factors, the states with lower spins can become the ground states. Along with such reversion of the total spin of the ground state, another kind of the vortices can be identified. As illustrated in Fig.5, in the states (-17,1,1) and (-17,1,0), there are not only the vortices similar to those in (-18,2,0) but also the

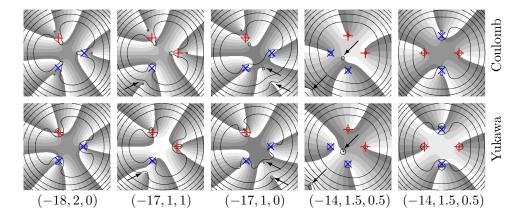


FIG. 5: (Color online) Spin-dependent vortex distributions of several states with long-range Coulomb (first row) and Yukawa screened interaction (second row). + and \times indicate the positions of pinned spin-up and -down electrons, respectively. The arrows indicate the separated vortices.

separated vortices which do not approach the positions of the electrons when the interaction is screened, as indicated by arrows in the plots. Such vortices, which keep separated from others and do not move to the infinity when the screened interaction is considered, are analogy of the quasi-particle in 2DEGs. An interesting feature is that the two states have different vortex distributions although they are degenerate in energy and have same total spin. In Fig.5, it can be seen that the vortex numbers of (-17,1,1) and (-17,1,0) are same as that of (-18,2,0) because they have same filling factor. For (-17,1,1), there is one separated vortex. The state (-17,1,0) has one more separated vortex than (-17,1,1). The reason is that the two identical spin-down electrons in (-17,1,0) must have same vortex number. So one of the vortices belonging to a spin-up electron of (-17,1,1) must leave the electron when it becomes spin-down. Similar differences of vortex distributions also exist in some other degenerate states with different S_z . In fact, these degenerate states also have different entanglement entropies, because both the vortex distribution and the entropy reflect the component differences between the states.

For five-electron case, there are also the separated vortex excitations. However, when we recognize the separated vortices by employing the screened interaction, it must be realized that the display of the behavior of a vortex may depend on the fixation manner of the pinned electron. The merging behavior of a vortex to the position of the electron may be only the result of the inspection from a particular 'viewpoint'. That is to say, only those merging behaviors irrespective to the fixation manner are true. We present an example in Fig.5. For the five-electron state (-14,0.5,0.5), the total vortex number in the plots is six. If the pinned electrons are in alternative mode, it seems that there are two vortices which can approach the position of the spin-down electron. But from the viewpoint of the neighbor mode, only one vortex does so, another one keeps separated from the electron. Then we can realize that the merging behavior is only

a false expression due to the particular 'viewpoint' and there are two separated vortices in (-14,0.5,0.5).

By making great effort on the classification of the vortices, now we can return to the analysis of the absent states in the angular momentum transitions. The behavior of the separated vortices implies that they have no use in reducing the short-range interaction between electrons. We know that the concentrated vortices in the Laughlin wave function are most efficient way to reduce the shortrange interaction. Then we see that when the short-range interaction becomes more and more important, there are vortices in the quantum dot which approach the Laughlin limit to reduce the interaction except the separated ones. From the tables in Appendix, we can find that most of the absent states have more separated vortices than neighbor states. For example, the separated vortex numbers of the four-electron absent state (-6,0,0) and all the five-electron absent states with S=0.5 exceed those of the neighbor states. Most of these absent states have no less than three separated vortices. In fact, more separated vortices make the vortex distribution of those states more dispersed than the neighbor ones and are unfavorable in energy when the short-range interaction is still important. Then those states may be absent in the transition sequences for the lowest states. The states with S unequal to the lowest value are more complicated. As discussed in Fig.5, the states with same L,S but different S_z can have different separated vortices. However, within the states with same S_z it can still be found that the absent states at least have more separated vortices than the neighbor states with smaller |L|. The only one special absent state is (-17,1.5,0.5). It has fewer vortices than the neighbor states and so few vortices also have no advantage in reducing the energy.

As mentioned previously, with the increase of the magnetic field, the electrons gradually form the rotating Wigner molecules. The short-range interaction becomes unimportant and the difference between separated and other vortices can be ignored. Then even the states with

more separated vortices are no longer unfavorable in energy and the absences of the states in the transition sequences gradually disappear. Besides this, the monotonicity of the vortex number in the angular momentum transition need not to be preserved. The data in the tables in Appendix also show these conclusions.

IV. SUMMARY

In summary, we have investigated the vortex structures of the electronic states in quantum dot without the Zeeman splitting. The vortex display with spin degree of freedom depends on both the choice of the probe electron and the fixation manner of the pinned electrons in the conditional single-particle wave function. By choosing an appropriate way to fix the pinned electrons in the functions we explore the transition patterns of the vortex number in magnetic fields for the lowest states with different spins. It is found that the vortex number increases monotonously when the field is not very strong and the states with certain angular momenta are absent from the transition sequences. When the field becomes strong, the absences disappear and the monotonicity may not be preserved. By examining the behaviors of the vortices with different range of the interaction between electrons, we can identify two kinds of vortices in the quantum dot which are respectively analogous to the vortices of the electrons and reversed-spin quasi-particles in the fractional quantum Hall system. The quasi-particlelike vortices do not approach the position of the electron when the interaction is screened and have no use in reducing the short-range interaction. Then the states with more such separated vortices are unfavorable in energy when the field is not very strong and may be absent from the transition sequences. These results imply that the understanding of the vortex structures and formations with spin degree of freedom are important for the studies and the control of the spin-relevant electronic states in nanostructures in magnetic fields.

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APPENDIX: VORTEX FOR THE LOWEST STATE WITH DIFFERENT SPINS

The vortex distributions with respect to all allowable angular momenta for the lowest states with different total spins are listed in the Tab.I and Tab.II. The columns 'total' are the total vortex numbers displayed by the conditional single-particle wave functions. The following three columns are respectively the vortices of per spin-up, per spin-down pinned electron and the separated vortices identified by the screened interaction.

TABLE I: Vortex numbers of the four-electron states with S=0 and 1 and $S_z=0$. The states marked with * are those absent from the transition sequences according to the results of the exact diagonalization.

S = 0					S=1					
$ L ^{\dagger}$	Vortex Number				$ L ^{\ddagger}$	Vortex Number				
	total	per ↑	$per \downarrow$	sep.	L	total	per ↑	$per \downarrow$	sep.	
2	1	1	0	0	3	2	1	0	1	
4	2	1	0	1	4	3	1	0	2	
6*	4	1	0	3	5	3	1	0	2	
					7	4	1	1	1	
8	4	1	1	1	8*	5	1	1	2	
10	5	1	2	0	9	5	1	1	2	
					11	6	1	1	3	
12	7	1	2	2	12	7	1	1	4	
14	7	3	2	0	13	8	1	1	5	
					15	8	3	2	1	
16	8	3	2	1	16	9	3	2	2	
18	10	3	3	1	17	9	3	2	2	
					19	10	3	3	1	
20	10	3	3	1	20	11	3	3	2	
22	11	3	4	0	21	11	3	3	2	
					23	13	3	3	4	
24	13	3	3	4	24	13	3	3	4	
26	13	5	4	0	25	14	4	4	2	
					27	14	5	4	1	
28	15	5	4	2	28	15	5	4	2	
30	16	5	5	1	29	15	5	4	2	

[†] L can be arbitrary even integer for the state with S=0

 $^{^{\}ddagger}$ L can be arbitrary integer but unequal to 4n+2 for the state with S=1

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TABLE II: Vortex numbers of the five-electron states with S=0.5 and 1.5 and $S_z=0.5$. The states marked with * are those absent from the transition sequences according to the results of the exact diagonalization.

S = 0.5					S = 1.5					
Vortey Number						Vontor Number				
$ L ^{\dagger}$	total				$ L ^{\ddagger}$				sep.	
4	2	1	0	0	4	2	1	0	0	
5	3	1	0	1						
6*	4	1	0	2	6	3	1	0	1	
7	3	1	0	1	7*	4	1	0	2	
8	4	1	0	2	8	4	1	0	2	
9*	5	1	0	3	9	4	1	0	2	
10*	5	1	0	3						
11*	6	1	0	4	11	5	1	1	1	
12	5	1	1	1	12*	6	1	1	2	
13	5	1	1	1	13*	6	1	1	2	
14*	7	1	1	3	14	6	1	1	2	
15	6	1	1	2						
16	6	1	1	2	16	8	1	1	4	
17*	7	1	1	3	17*	7	1	1	3	
18*	8	1	1	4	18	9	1	2	3	
19	9	1	2	3	19*	10	1	2	4	
20*	10	1	2	4						
21	9	1	2	3	21*	10	1	2	4	
22*	10	1	2	4	22	10	1	2	4	
23*	11	1	2	5	23	11	3	2	1	
24	10	3	2	0	24*	11	1	1	7	
25*	11	2	2	3						
26	12	3	2	2	26	11	3	2	1	
27	11	3	2	1	27	12	3	2	2	
28	12	3	2	2	28	12	3	2	2	
29*	13	3	2	3	29	12	3	2	2	
30	13	3	3	1						
31*	14	3	3	2	31	13	3	3	1	
32	12	3	3	0	32	13	3	3	1	
33	13	3	3	1	33	14	3	3	2	
34*	14	3	3	2	34	14	3	3	2	
35	14	3	3	2						
36	14	3	3	2	36	15	3	3	3	
37	15	3	4	1	37	17	4	3	3	
38	16	4	3	2	38	17	3	3	5	
39	17	3	4	3	39	18	4	4	2	
40	18	3	4	4						
41	17	3	4	3	41	18	4	4	2	
42	18	4	4	2	42	18	3	4	4	
43	19	3	5	3	43	19	4	4	3	
44	18	5	4	0	44	19	4	4	3	
45	19	4	4	3						
46	20	5	4	2	46	20	5	4	2	
47	19	4	4	3	47	20	5	4	2	
48	20	5	4	2	48	21	5	5	1	
49	21	5	4	3	49	21	5	5	1	
50	21	5	5	1						

 $^{^\}dagger$ L can be arbitrary integer for the state with S=0.5

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 $^{^{\}ddagger}$ L can be arbitrary integer but unequal to 5n for the state with S=1.5